OpenMP* 4.0 for HPC in a Nutshell

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<table>
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OpenMP API

• De-facto standard, OpenMP 4.0 out since July 2013

• API for C/C++ and Fortran for shared-memory parallel programming

• Based on directives (pragmas in C/C++)

• Portable across vendors and platforms

• Supports various types of parallelism
# Evolution of Hardware (at Intel)

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Core(s) up to</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>6</td>
<td>8</td>
<td>12</td>
<td>18</td>
<td>61</td>
</tr>
<tr>
<td>Threads up to</td>
<td>2</td>
<td>2</td>
<td>8</td>
<td>12</td>
<td>16</td>
<td>24</td>
<td>36</td>
<td>244</td>
</tr>
<tr>
<td>SIMD Width (bits)</td>
<td>128</td>
<td>128</td>
<td>128</td>
<td>128</td>
<td>256</td>
<td>256</td>
<td>256</td>
<td>512</td>
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</table>

*(die sizes not to scale, for illustration only)*

Product specification for launched and shipped products available on ark.intel.com.

1 Not launched or in planning.
# Levels of Parallelism in OpenMP 4.0

<table>
<thead>
<tr>
<th>Level</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cluster</td>
<td>Group of computers communicating through fast interconnect</td>
</tr>
<tr>
<td>Coprocessors/Accelerators</td>
<td>Special compute devices attached to the local node through special interconnect</td>
</tr>
<tr>
<td>Node</td>
<td>Group of processors communicating through shared memory</td>
</tr>
<tr>
<td>Socket</td>
<td>Group of cores communicating through shared cache</td>
</tr>
<tr>
<td>Core</td>
<td>Group of functional units communicating through registers</td>
</tr>
<tr>
<td>Hyper-Threads</td>
<td>Group of thread contexts sharing functional units</td>
</tr>
<tr>
<td>Superscalar</td>
<td>Group of instructions sharing functional units</td>
</tr>
<tr>
<td>Pipeline</td>
<td>Sequence of instructions sharing functional units</td>
</tr>
<tr>
<td>Vector</td>
<td>Single instruction using multiple functional units</td>
</tr>
</tbody>
</table>

**OpenMP 4.0 for Devices**

**OpenMP 4.0 Affinity**

**OpenMP 4.0 SIMD**
#pragma omp parallel
{
    #pragma omp for
    for (i = 0; i < N; i++)
    {
        ...
    }

    #pragma omp for
    for (i = 0; i < N; i++)
    {
        ...
    }
}

fork

distribute work

barrier

barrier

distribute work

join
double a[N];
double l,s = 0;

#pragma omp parallel for reduction(+:s) private(l) \\
schedule(static,4)
for (i = 0; i<N; i++)
{
    l = log(a[i]);
    s += l;
}

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OpenMP Intro in Three Slides (3)

```c
#pragma omp parallel
#pragma omp single
for (e = l->first; e; e = e->next)
    #pragma omp task
    process(e);
```
OpenMP 4.0 SIMD
In a Time before OpenMP 4.0

- Programmers had to rely on auto-vectorization...
- ... or to use vendor-specific extensions
  - Programming models (e.g., Intel® Cilk™ Plus)
  - Compiler pragmas (e.g., #pragma vector)
  - Low-level constructs (e.g., _mm_add_pd())

```c
#pragma omp parallel for
#pragma vector always
#pragma ivdep
for (int i = 0; i < N; i++) {
    a[i] = b[i] + ...;
}
```

You need to trust the compiler to do the “right” thing.
OpenMP SIMD Loop Construct

- Vectorize a loop nest
  - Cut loop into chunks that fit a SIMD vector register
  - No parallelization of the loop body

- **Syntax (C/C++)**
  ```c
  #pragma omp simd [clause[[,] clause],...]
  for-loops
  ```

- **Syntax (Fortran)**
  ```fortran
  !$omp simd [clause[[,] clause],...]
  do-loops
  ```
Example

```c
void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
    #pragma omp simd reduction(+:sum)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}
```
Data Sharing Clauses

• **private(var-list):**
  Uninitialized vectors for variables in var-list

• **firstprivate(var-list):**
  Initialized vectors for variables in var-list

• **reduction(op:var-list):**
  Create private variables for var-list and apply reduction operator op at the end of the construct
SIMD Loop Clauses

- **safelen (length)**
  - Maximum number of iterations that can run concurrently without breaking a dependence
  - In practice, maximum vector length
- **linear (list[:linear-step])**
  - The variable’s value is in relationship with the iteration number
    \[ x_i = x_{\text{orig}} + i \times \text{linear-step} \]
- **aligned (list[:alignment])**
  - Specifies that the list items have a given alignment
  - Default is alignment for the architecture
- **collapse (n)**
Loop-Carried Dependencies

- Dependencies may occur across loop iterations
  - Loop-carried dependency
- The following code contains such a dependency:

```c
void lcd_ex(float* a, float* b, size_t n, float c1, float c2) {
    size_t i;
    for (i = 0; i < n; i++) {
        a[i] = c1 * a[i + 17] + c2 * b[i];
    }
}
```

- Some iterations of the loop have to complete before the next iteration can run
  - Simple trick: can you reverse the loop w/o getting wrong results?
Loop-Carried Dependencies

• Can we parallelize or vectorize the loop?
  • Parallelization: no
    (except for very specific loop schedules)
  • Vectorization: yes
    (if vector length is shorter than any distance of any dependency)
SIMD Worksharing Construct

- Parallelize and vectorize a loop nest
  - Distribute a loop’s iteration space across a thread team
  - Subdivide loop chunks to fit a SIMD vector register

- Syntax (C/C++)
  
  ```c
  #pragma omp for simd [clause[[,] clause],...] for-loops
  ```

- Syntax (Fortran)
  
  ```fortran
  !$omp do simd [clause[[,] clause],...] do-loops
  ```
void sprod(float *a, float *b, int n) {
    float sum = 0.0f;
#pragma omp for simd reduction(+:sum)
    for (int k=0; k<n; k++)
        sum += a[k] * b[k];
    return sum;
}
SIMD Function Vectorization

```c
float min(float a, float b) {
    return a < b ? a : b;
}

float distsq(float x, float y) {
    return (x - y) * (x - y);
}

void example() {
    #pragma omp parallel for simd
    for (i=0; i<N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
    }
}
```
SIMD Function Vectorization

- Declare one or more functions to be compiled for calls from a SIMD-parallel loop

- Syntax (C/C++):
  
  ```
  #pragma omp declare simd [clause[[], clause],...]
  [#pragma omp declare simd [clause[[], clause],...]]
  [...] function-definition-or-declaration
  ```

- Syntax (Fortran):
  
  ```
  !$omp declare simd (proc-name-list)
  ```
SIMD Function Vectorization

```c
#pragma omp declare simd
float min(float a, float b) {
    return a < b ? a : b;
}

#pragma omp declare simd
float distsq(float x, float y) {
    return (x - y) * (x - y);
}

void example() {
    #pragma omp parallel for simd
    for (i=0; i<N; i++) {
        d[i] = min(distsq(a[i], b[i]), c[i]);
    }
}

vec8 min_v(vec8 a, vec8 b) {
    return a < b ? a : b;
}

vec8 distsq_v(vec8 x, vec8 y) {
    return (x - y) * (x - y);
}

vd = min_v(distsq_v(va, vb, vc))
```
SIMD Function Vectorization

- **simdlen** *(length)*
  - generate function to support a given vector length
- **uniform** *(argument-list)*
  - argument has a constant value between the iterations of a given loop
- **inbranch**
  - function always called from inside an if statement
- **notinbranch**
  - function never called from inside an if statement
- **linear** *(argument-list[:linear-step])*
- **aligned** *(argument-list[:alignment])*  
- **reduction** *(operator:list)*

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OpenMP 4.0 for Devices
Device Model

- OpenMP 4.0 supports accelerators/coprocessors
- Device model:
  - One host
  - Multiple accelerators/coprocessors of the same kind
OpenMP 4.0 for Devices - Constructs

• Transfer control [and data] from the host to the device

• Syntax (C/C++)
  #pragma omp target [data] [clause[[], clause],...]
  structured-block

• Syntax (Fortran)
  !$omp target [data] [clause[[], clause],...]
  structured-block
  !$omp end target [data]

• Clauses
  device(scalar-integer-expression)
  map(alloc | to | from | tofrom: list)
  if(scalar-expr)
Execution Model

• The **target construct** transfers the control flow to the target device
  • Transfer of control is sequential and synchronous
  • The transfer clauses control direction of data flow
  • Array notation is used to describe array length
• The **target data** construct creates a scoped device data environment
  • Does not include a transfer of control
  • The transfer clauses control direction of data flow
  • The device data environment is valid through the lifetime of the target data region
• **Use target update** to request data transfers from within a target data region
Execution Model

- Data environment is lexically scoped
  - Data environment is destroyed at closing curly brace
  - Allocated buffers/data are automatically released
Example

```c
#pragma omp target data device(0) map(aloc:tmp[:N]) map(to:input[:N]) map(from:res)
{
    #pragma omp target device(0)
    #pragma omp parallel for
    for (i=0; i<N; i++)
        tmp[i] = some_computation(input[i], i);

    update_input_array_on_the_host(input);

    #pragma omp target update device(0) to(input[:N])

    #pragma omp target device(0)
    #pragma omp parallel for reduction(+:res)
    for (i=0; i<N; i++)
        res += final_computation(input[i], tmp[i], i)
}
```
teams Construct

- Support multi-level parallel devices

- Syntax (C/C++):
  
  ```
  #pragma omp teams [clause[[,] clause],...]
  structured-block
  ```

- Syntax (Fortran):
  
  ```
  !$omp teams [clause[[,] clause],...]
  structured-block
  ```

- Clauses
  
  ```
  num_teams(integer-expression)
  num_threads(integer-expression)
  default(shared | none)
  private(list), firstprivate(list)
  shared(list), reduction(operator : list)
  ```
Offloading SAXPY to a Coprocessor

```c
int main(int argc, const char* argv[]) {
    float *x = (float*) malloc(n * sizeof(float));
    float *y = (float*) malloc(n * sizeof(float));
    // Define scalars n, a, b & initialize x, y

    #pragma omp target data map(to:x[0:n])
    {
        #pragma omp target map(tofrom:y)
        #pragma omp teams num_teams(num_blocks) num_threads(nthreads)

        for (int i = 0; i < n; i += num_blocks) {
            for (int j = i; j < i + num_blocks; j++) {
                y[j] = a*x[j] + y[j];
            }
        }
    }
    free(x); free(y); return 0;
}
```

---

*all do the same*
Offloading SAXPY to a Coprocessor

```c
int main(int argc, const char* argv[]) {
    float *x = (float*) malloc(n * sizeof(float));
    float *y = (float*) malloc(n * sizeof(float));
    // Define scalars n, a, b & initialize x, y

    #pragma omp target data map(to:x[0:n])
    {
        #pragma omp target map(tofrom:y)
        #pragma omp teams num_teams(num blocks) num_threads(bsize)
        #pragma omp distribute
        for (int i = 0; i < n; i += num_blocks){
            #pragma omp parallel for
            for (int j = i; j < i + num_blocks; j++) {
                y[j] = a*x[j] + y[j];
            }
        }
        free(x);
        free(y);
    }
    return 0; }
```
Offloading SAXPY to a Coprocessor

```c
int main(int argc, const char* argv[]) {
    float *x = (float*) malloc(n * sizeof(float));
    float *y = (float*) malloc(n * sizeof(float));
    // Define scalars n, a, b & initialize x, y
    #pragma omp target map(to:x[0:n]) map(tofrom:y)
    {
        #pragma omp teams distribute parallel for 
        num_teams(num_blocks) num_threads(bsize)
        for (int i = 0; i < n; ++i){
            y[i] = a*x[i] + y[i];
        }
    }
    free(x); free(y); return 0;
}
```
OpenMP 4.0 Affinity
NUMA is here to Stay...

- (Almost) all multi-socket compute servers are NUMA systems
  - Different access latencies for different memory locations
  - Different bandwidth observed for different memory locations
- Example: Intel® Xeon E5-2600v2 Series processor
Thread Affinity – Why It Matters?

STREAM Triad, Intel® Xeon E5-2697v2

GB/sec [higher is better]

# of threads/cores

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

- compact, par
- scatter, par
- compact, seq
- scatter, seq
Thread Affinity – Processor Binding

Binding strategies depend on the machine and the application.

- **Putting threads far, i.e. on different packages**
  - (May) improve the aggregated memory bandwidth
  - (May) improve the combined cache size
  - (May) decrease performance of synchronization constructs

- **Putting threads close together, i.e. on two adjacent cores which possibly share the cache**
  - (May) improve performance of synchronization constructs
  - (May) decrease the available memory bandwidth and cache size (per thread)
Thread Affinity in OpenMP* 4.0

- OpenMP 4.0 introduces the concept of places...
  - set of threads running on one or more processors
  - can be defined by the user
  - pre-defined places available:
    - threads  one place per hyper-thread
    - cores    one place exists per physical core
    - sockets  one place per processor package

... and affinity policies...
- spread   spread OpenMP threads evenly among the places
- close     pack OpenMP threads near master thread
- master    collocate OpenMP thread with master thread

... and means to control these settings
- Environment variables OMP_PLACES and OMP_PROC_BIND
- clause proc_bind for parallel regions
Thread Affinity Example

- Example (Intel® Xeon Phi™ Coprocessor): Distribute outer region, keep inner regions close

OMP_PLACES=cores(8); OMP_NUM_THREADS=4,4

#pragma omp parallel proc_bind(spread)
#pragma omp parallel proc_bind(close)
We’re Almost Through

• This presentation focused on HPC stuff

• OpenMP 4.0 has more to offer!
  • Improved Fortran 2003 support
  • User-defined reductions
  • Task dependencies
  • Cancellation

• We can chat about these features during the Q&A (if you want to)
The last Slide...

- OpenMP 4.0 is a major leap for OpenMP
  - New kind of parallelism has been introduced
  - Support for heterogeneous systems with coprocessor devices

- Support in Intel® Composer XE 2013 SP1
  - SIMD Constructs (except combined constructs)
  - OpenMP for devices (except combined constructs)
  - OpenMP Affinity